

1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydro-pyrimidin-5-yl]ethanone

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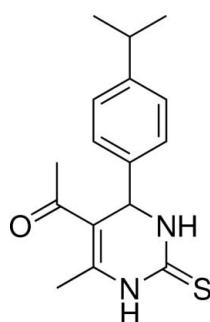
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Key indicators: single-crystal X-ray study; $T = 123\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 15.8.

In the title molecule, $\text{C}_{16}\text{H}_{20}\text{N}_2\text{OS}$, the heterocyclic ring adopts a slightly distorted flattened boat conformation, and the plane through the four coplanar atoms makes a dihedral angle of $86.98(6)^\circ$ with the benzene ring. The thione, acetyl and methyl groups lie on the opposite side of the heterocyclic mean plane to the isopropylphenyl group which has an axial orientation. A weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond is observed. In the crystal, molecules are linked via $\text{N}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{S}$ and $\text{C}-\text{H}\cdots\text{S}$ hydrogen bonds.

Related literature

For chemical and biological applications and for the closely related crystal structures of the chloro and fluoro derivatives, see: Anuradha *et al.* (2009, 2012).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{20}\text{N}_2\text{OS}$	$V = 3100.62(10)\text{ \AA}^3$
$M_r = 288.41$	$Z = 8$
Monoclinic, $C2/c$	$\text{Cu } K\alpha$ radiation
$a = 26.8413(5)\text{ \AA}$	$\mu = 1.83\text{ mm}^{-1}$
$b = 9.5657(2)\text{ \AA}$	$T = 123\text{ K}$
$c = 12.0764(2)\text{ \AA}$	$0.49 \times 0.23 \times 0.18\text{ mm}$
$\beta = 90.370(2)^\circ$	

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer	5607 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2012)	3042 independent reflections
$T_{\min} = 0.831$, $T_{\max} = 1.000$	2776 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$\Delta\rho_{\text{max}} = 0.42\text{ e \AA}^{-3}$
$S = 1.05$	$\Delta\rho_{\text{min}} = -0.39\text{ e \AA}^{-3}$
3042 reflections	
193 parameters	

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1 \cdots O5 ⁱ	0.83 (2)	2.12 (2)	2.9445 (17)	174 (2)
N3—H3 \cdots S2 ⁱⁱ	0.840 (19)	2.56 (2)	3.3481 (13)	156.9 (18)
C61—H61A \cdots O5 ⁱ	0.98	2.22	2.9148 (19)	127
C61—H61B \cdots S2 ⁱⁱⁱ	0.98	2.86	3.7145 (16)	146

Symmetry codes: (i) $x, -y + 1, z - \frac{1}{2}$; (ii) $-x, -y, -z$; (iii) $-x, -y + 1, -z$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2487).

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supplementary materials

Acta Cryst. (2012). E68, o2641 [doi:10.1107/S1600536812034046]

1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydro-pyrimidin-5-yl]ethanone

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Comment

As part of our investigations of dihydropyrimidine derivatives (Anuradha *et al.*, 2009, 2012) to compare their chemical and biological activities, we have undertaken the X-ray crystal structure analysis of the title compound.

In the title molecule, $C_{16}H_{20}N_2OS$ (Fig. 1), the heterocyclic ring adopts a slightly distorted flattened boat conformation, and the plane through the four coplanar atoms (C2, N3, C5 and C6) makes a dihedral angle of $86.98(6)^\circ$ with the benzene ring. The thione, acetyl and methyl groups have equatorial orientations with respect to the attached heterocyclic ring, whereas the isopropylphenyl group has an axial orientation.

Intermolecular N1—H1···O51, N3—H3···S2 and C61—H61B···S2 hydrogen bonds are found in the crystal structure. A weak intramolecular C61—H61A···O51 hydrogen bond is also observed (Fig. 2, Table 1).

Experimental

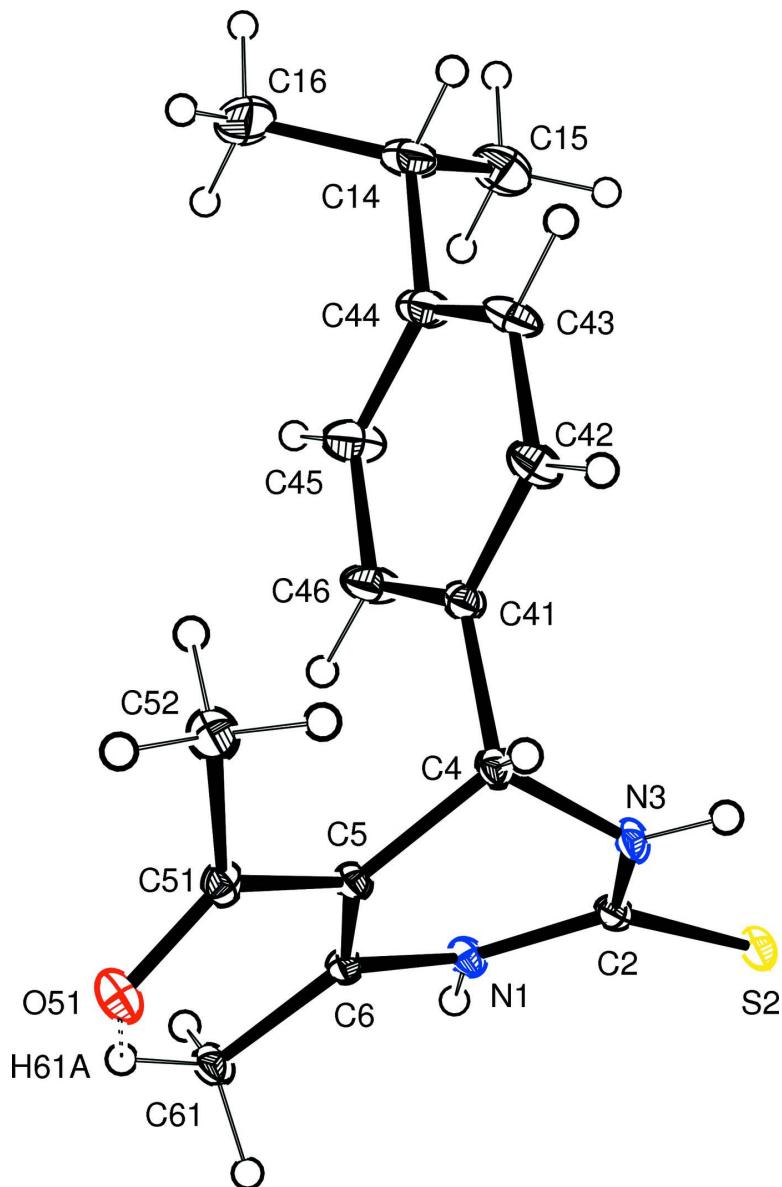
A solution of acetylacetone (1.0012 g, 0.01 mol), 4-isopropylbenzaldehyde (1.48 g, 0.01 mol) and thiourea (1.14 g, 0.015 mol) was heated under reflux in the presence of calcium fluoride (0.07 g, 0.001 mol) for 2 h (monitored by TLC). After completion of the reaction, the reaction mixture was cooled to room temperature and poured into crushed ice. The solid product was filtered under suction and purified by recrystallization from hot methanol to give the product in pure form. Yield 1.86 g (93%).

Refinement

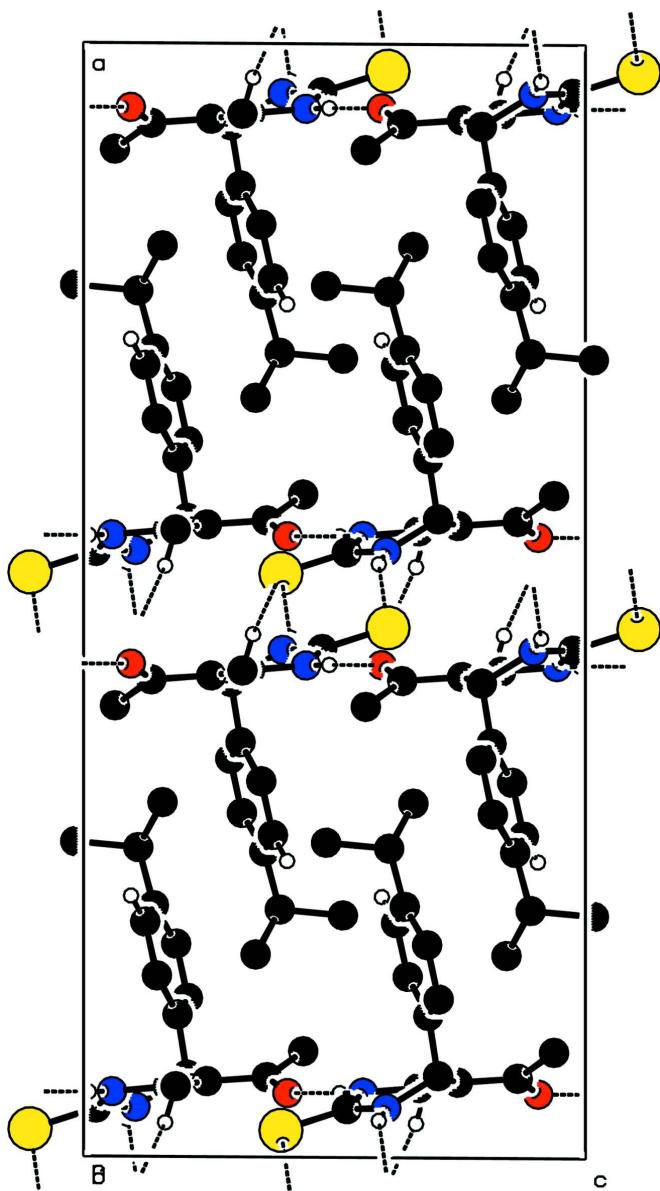
The two N-bound H atoms were located in a difference Fourier map and refined freely; N1—H1 = 0.83 (2) Å and N3—H3 = 0.840 (19) Å. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with Csp^2 —H = 0.95, C(methyl)—H = 0.98, and C(methine)—H = 1.00 Å; $U_{iso}(H) = kU_{eq}(C)$, where $k = 1.5$ for methyl H and 1.2 for all other H atoms.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius. Dashed lines indicate the intramolecular C—H···O hydrogen bond.

**Figure 2**

The packing of the title compound, viewed down the b axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidin-5-yl]ethanone

Crystal data

$C_{16}H_{20}N_2OS$

$M_r = 288.41$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 26.8413 (5) \text{ \AA}$

$b = 9.5657 (2) \text{ \AA}$

$c = 12.0764 (2) \text{ \AA}$

$\beta = 90.370 (2)^\circ$

$V = 3100.62 (10) \text{ \AA}^3$

$Z = 8$

$F(000) = 1232$

$D_x = 1.236 \text{ Mg m}^{-3}$

Melting point: 486 K

Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$

Cell parameters from 3841 reflections

$\theta = 3.3\text{--}73.5^\circ$

$\mu = 1.83 \text{ mm}^{-1}$
 $T = 123 \text{ K}$

Prism, colourless
 $0.49 \times 0.23 \times 0.18 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
 Radiation source: Enhance (Cu) X-ray Source
 Graphite monochromator
 Detector resolution: 10.5081 pixels mm^{-1}
 ω scans
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
 $T_{\min} = 0.831$, $T_{\max} = 1.000$

5607 measured reflections
 3042 independent reflections
 2776 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\max} = 73.6^\circ$, $\theta_{\min} = 3.3^\circ$
 $h = -30 \rightarrow 33$
 $k = -11 \rightarrow 10$
 $l = -10 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.113$
 $S = 1.05$
 3042 reflections
 193 parameters
 0 restraints
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring sites
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 1.9078P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S2	0.02408 (1)	0.17969 (4)	-0.10663 (3)	0.0195 (1)
O51	0.05759 (4)	0.41789 (12)	0.40606 (9)	0.0236 (3)
N1	0.05834 (5)	0.34011 (14)	0.05675 (10)	0.0163 (3)
N3	0.04445 (5)	0.11271 (13)	0.10324 (10)	0.0174 (3)
C2	0.04342 (5)	0.20984 (16)	0.02461 (12)	0.0157 (4)
C4	0.07362 (5)	0.12832 (15)	0.20639 (12)	0.0163 (4)
C5	0.06781 (5)	0.27819 (15)	0.24566 (12)	0.0148 (4)
C6	0.06273 (5)	0.37919 (15)	0.16783 (12)	0.0154 (4)
C14	0.27761 (7)	-0.0514 (2)	0.10895 (16)	0.0335 (6)
C15	0.28259 (8)	-0.0600 (2)	-0.01678 (18)	0.0417 (7)
C16	0.31816 (8)	0.0428 (3)	0.1572 (2)	0.0553 (8)
C41	0.12759 (6)	0.08478 (16)	0.18712 (12)	0.0184 (4)
C42	0.14242 (7)	-0.05178 (17)	0.20769 (14)	0.0255 (5)
C43	0.19116 (7)	-0.09414 (18)	0.18449 (15)	0.0294 (5)

C44	0.22550 (6)	-0.00268 (19)	0.14005 (14)	0.0268 (5)
C45	0.21077 (7)	0.1352 (2)	0.12272 (17)	0.0336 (6)
C46	0.16255 (7)	0.17846 (18)	0.14600 (16)	0.0295 (5)
C51	0.07174 (5)	0.30757 (16)	0.36521 (12)	0.0172 (4)
C52	0.09518 (7)	0.19628 (17)	0.43753 (13)	0.0238 (4)
C61	0.06312 (6)	0.53426 (16)	0.18341 (13)	0.0205 (4)
H1	0.0578 (8)	0.404 (2)	0.0103 (18)	0.027 (5)*
H3	0.0331 (8)	0.033 (2)	0.0883 (16)	0.022 (5)*
H4	0.05908	0.06499	0.26360	0.0195*
H14	0.28252	-0.14749	0.13978	0.0401*
H15A	0.25674	-0.12199	-0.04673	0.0625*
H15B	0.31551	-0.09716	-0.03547	0.0625*
H15C	0.27872	0.03349	-0.04881	0.0625*
H16A	0.31439	0.13744	0.12736	0.0829*
H16B	0.35096	0.00585	0.13732	0.0829*
H16C	0.31517	0.04545	0.23804	0.0829*
H42	0.11939	-0.11679	0.23764	0.0305*
H43	0.20084	-0.18777	0.19963	0.0353*
H45	0.23407	0.20068	0.09452	0.0403*
H46	0.15335	0.27312	0.13370	0.0353*
H52A	0.09405	0.22594	0.51515	0.0357*
H52B	0.12992	0.18230	0.41561	0.0357*
H52C	0.07678	0.10845	0.42872	0.0357*
H61A	0.07008	0.55610	0.26127	0.0308*
H61B	0.03056	0.57263	0.16234	0.0308*
H61C	0.08898	0.57568	0.13681	0.0308*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S2	0.0271 (2)	0.0143 (2)	0.0171 (2)	0.0000 (1)	-0.0027 (1)	-0.0011 (1)
O51	0.0312 (6)	0.0183 (6)	0.0212 (5)	0.0007 (5)	0.0029 (4)	-0.0047 (4)
N1	0.0205 (6)	0.0117 (6)	0.0168 (6)	0.0001 (5)	0.0005 (5)	0.0016 (5)
N3	0.0226 (6)	0.0101 (6)	0.0194 (6)	-0.0027 (5)	-0.0022 (5)	-0.0006 (5)
C2	0.0159 (7)	0.0132 (7)	0.0181 (7)	0.0017 (5)	0.0011 (5)	-0.0003 (5)
C4	0.0190 (7)	0.0129 (7)	0.0169 (7)	-0.0008 (5)	-0.0005 (5)	0.0009 (5)
C5	0.0143 (6)	0.0123 (7)	0.0179 (7)	0.0000 (5)	0.0005 (5)	-0.0011 (5)
C6	0.0123 (6)	0.0145 (7)	0.0195 (7)	0.0000 (5)	0.0009 (5)	-0.0023 (5)
C14	0.0285 (9)	0.0315 (10)	0.0404 (10)	0.0150 (8)	0.0036 (7)	-0.0022 (8)
C15	0.0407 (11)	0.0405 (12)	0.0440 (11)	0.0109 (9)	0.0115 (9)	-0.0081 (9)
C16	0.0253 (10)	0.0666 (16)	0.0738 (16)	0.0188 (10)	-0.0064 (10)	-0.0274 (13)
C41	0.0212 (7)	0.0157 (7)	0.0183 (7)	0.0032 (6)	-0.0008 (5)	-0.0001 (5)
C42	0.0310 (8)	0.0164 (8)	0.0291 (8)	0.0032 (7)	0.0035 (6)	0.0025 (6)
C43	0.0355 (9)	0.0177 (8)	0.0351 (9)	0.0121 (7)	0.0026 (7)	0.0021 (7)
C44	0.0258 (8)	0.0260 (9)	0.0286 (8)	0.0099 (7)	0.0008 (6)	-0.0015 (7)
C45	0.0250 (8)	0.0262 (10)	0.0497 (11)	0.0050 (7)	0.0091 (7)	0.0095 (8)
C46	0.0240 (8)	0.0187 (9)	0.0458 (11)	0.0059 (7)	0.0065 (7)	0.0080 (7)
C51	0.0154 (7)	0.0163 (7)	0.0198 (7)	-0.0041 (5)	0.0014 (5)	0.0006 (5)
C52	0.0312 (8)	0.0216 (8)	0.0186 (7)	0.0011 (7)	-0.0026 (6)	0.0019 (6)
C61	0.0268 (8)	0.0130 (7)	0.0218 (7)	0.0025 (6)	-0.0021 (6)	0.0001 (6)

Geometric parameters (\AA , $^{\circ}$)

S2—C2	1.6894 (15)	C45—C46	1.389 (3)
O51—C51	1.2262 (19)	C51—C52	1.512 (2)
N1—C2	1.365 (2)	C4—H4	1.0000
N1—C6	1.3968 (19)	C14—H14	1.0000
N3—C2	1.3287 (19)	C15—H15A	0.9800
N3—C4	1.4746 (19)	C15—H15B	0.9800
N1—H1	0.83 (2)	C15—H15C	0.9800
N3—H3	0.840 (19)	C16—H16A	0.9800
C4—C41	1.527 (2)	C16—H16B	0.9800
C4—C5	1.518 (2)	C16—H16C	0.9800
C5—C51	1.474 (2)	C42—H42	0.9500
C5—C6	1.354 (2)	C43—H43	0.9500
C6—C61	1.495 (2)	C45—H45	0.9500
C14—C44	1.524 (2)	C46—H46	0.9500
C14—C15	1.527 (3)	C52—H52A	0.9800
C14—C16	1.526 (3)	C52—H52B	0.9800
C41—C46	1.392 (2)	C52—H52C	0.9800
C41—C42	1.388 (2)	C61—H61A	0.9800
C42—C43	1.400 (3)	C61—H61B	0.9800
C43—C44	1.382 (2)	C61—H61C	0.9800
C44—C45	1.392 (3)		
C2—N1—C6	122.71 (13)	C41—C4—H4	108.00
C2—N3—C4	122.78 (12)	C15—C14—H14	108.00
C6—N1—H1	117.0 (14)	C16—C14—H14	108.00
C2—N1—H1	118.5 (14)	C44—C14—H14	108.00
C2—N3—H3	118.4 (13)	C14—C15—H15A	109.00
C4—N3—H3	117.6 (14)	C14—C15—H15B	109.00
N1—C2—N3	115.51 (13)	C14—C15—H15C	109.00
S2—C2—N3	123.78 (12)	H15A—C15—H15B	109.00
S2—C2—N1	120.71 (11)	H15A—C15—H15C	109.00
N3—C4—C41	110.05 (12)	H15B—C15—H15C	109.00
C5—C4—C41	113.87 (12)	C14—C16—H16A	109.00
N3—C4—C5	107.72 (11)	C14—C16—H16B	109.00
C4—C5—C6	117.84 (13)	C14—C16—H16C	109.00
C4—C5—C51	118.63 (12)	H16A—C16—H16B	110.00
C6—C5—C51	123.37 (13)	H16A—C16—H16C	109.00
N1—C6—C61	112.76 (13)	H16B—C16—H16C	109.00
C5—C6—C61	128.30 (14)	C41—C42—H42	120.00
N1—C6—C5	118.89 (13)	C43—C42—H42	120.00
C15—C14—C16	110.16 (17)	C42—C43—H43	119.00
C15—C14—C44	110.36 (16)	C44—C43—H43	119.00
C16—C14—C44	112.27 (16)	C44—C45—H45	119.00
C42—C41—C46	118.48 (16)	C46—C45—H45	120.00
C4—C41—C42	120.06 (14)	C41—C46—H46	120.00
C4—C41—C46	121.43 (14)	C45—C46—H46	120.00
C41—C42—C43	120.28 (16)	C51—C52—H52A	109.00
C42—C43—C44	121.41 (16)	C51—C52—H52B	109.00

C14—C44—C43	121.18 (16)	C51—C52—H52C	109.00
C14—C44—C45	120.86 (16)	H52A—C52—H52B	109.00
C43—C44—C45	117.95 (16)	H52A—C52—H52C	109.00
C44—C45—C46	121.05 (17)	H52B—C52—H52C	109.00
C41—C46—C45	120.78 (16)	C6—C61—H61A	109.00
O51—C51—C52	120.17 (13)	C6—C61—H61B	109.00
C5—C51—C52	117.29 (13)	C6—C61—H61C	109.00
O51—C51—C5	122.53 (13)	H61A—C61—H61B	109.00
N3—C4—H4	108.00	H61A—C61—H61C	109.00
C5—C4—H4	108.00	H61B—C61—H61C	109.00
C6—N1—C2—S2	163.66 (11)	C51—C5—C6—C61	4.0 (2)
C6—N1—C2—N3	-15.1 (2)	C4—C5—C51—O51	-164.54 (13)
C2—N1—C6—C5	21.1 (2)	C4—C5—C51—C52	16.63 (19)
C2—N1—C6—C61	-161.20 (13)	C6—C5—C51—O51	20.2 (2)
C4—N3—C2—S2	162.66 (11)	C6—C5—C51—C52	-158.59 (14)
C4—N3—C2—N1	-18.6 (2)	C15—C14—C44—C43	107.02 (19)
C2—N3—C4—C5	41.10 (18)	C15—C14—C44—C45	-71.9 (2)
C2—N3—C4—C41	-83.58 (17)	C16—C14—C44—C43	-129.67 (19)
N3—C4—C5—C6	-32.96 (17)	C16—C14—C44—C45	51.4 (2)
N3—C4—C5—C51	151.56 (12)	C4—C41—C42—C43	176.53 (15)
C41—C4—C5—C6	89.38 (16)	C46—C41—C42—C43	-1.7 (2)
C41—C4—C5—C51	-86.10 (15)	C4—C41—C46—C45	-176.17 (16)
N3—C4—C41—C42	-92.42 (16)	C42—C41—C46—C45	2.0 (3)
N3—C4—C41—C46	85.75 (17)	C41—C42—C43—C44	-0.5 (3)
C5—C4—C41—C42	146.53 (14)	C42—C43—C44—C14	-176.54 (16)
C5—C4—C41—C46	-35.3 (2)	C42—C43—C44—C45	2.4 (3)
C4—C5—C6—N1	5.98 (19)	C14—C44—C45—C46	176.88 (18)
C4—C5—C6—C61	-171.27 (13)	C43—C44—C45—C46	-2.1 (3)
C51—C5—C6—N1	-178.77 (13)	C44—C45—C46—C41	-0.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O51 ⁱ	0.83 (2)	2.12 (2)	2.9445 (17)	174 (2)
N3—H3···S2 ⁱⁱ	0.840 (19)	2.56 (2)	3.3481 (13)	156.9 (18)
C61—H61A···O51	0.98	2.22	2.9148 (19)	127
C61—H61B···S2 ⁱⁱⁱ	0.98	2.86	3.7145 (16)	146

Symmetry codes: (i) $x, -y+1, z-1/2$; (ii) $-x, -y, -z$; (iii) $-x, -y+1, -z$.